U.S. DEPARTMENT OF COMMERCE
National Technical Information Service

PB-280 788

A Highway Model for the Advection, Diffusion and Chemical Reaction of Pollutants Released by Automobiles Part I. Advection and Diffusion of SF6 Tracer Gas

Environmental Sciences Resarch Lab., Research Triangle Park, N C

1977

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/J-77-118	2. JOURNAL ARTICLE
3. R	PB 280 788
4. TITLE AND SUBTITLE A HIGHWAY MODEL FOR THE ADVECTION, DIFFUSION AND CHEMICAL REACTION OF POLLUTANTS RELEASED BY AUTOMOBILES: PART I- Advection And Diffusion Of SF_6 Tracer Gas	5. REPORT DATE
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Robert E. Eskridge and Kenneth L. Demerjian	8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS (Same as Box 12)	10. PROGRAM ELEMENT NO. 1AA603 AB-15 (FY-77)
	11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Environmental Sciences Research Laboratory - RTP, NC Office of Research and Development U.S. Environmental Protection Agency Research Triangle Park, NC 27711	13. TYPE OF REPORT AND PERIOD COVERED
	14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES REFERENCE: In: Preprint Volume, Joint Conference on Applications on Air Pollution Meteorology, Salt Lake City, UT. Boston, American Meteorological Society, 1977, p. 337-342.

16. ABSTRACT

A two-dimensional, finite-difference model simulating a highway has been developed which is able to handle linear and nonlinear chemical reactions.

Transport of the pollutants is accomplished by use of an upstream-flux-corrected algorithm developed at the Naval Research Laboratories. This algorithm insures positive concentrations and reduces numerical diffusion.

The model develops background eddy diffusion coefficients which are then perturbed by the mechanical turbulence introduced by vehicular motion.

The model calculations are compared to the SF_6 experiments carried out by General Motors in the GM sulfate dispersion experiment. Model predictions are compared to observations at each of the twenty observation points for all the experiments. The observations and predictions are correlated for each half hour period, and scatter diagrams presented. A discussion of the results and additional statistical comparisons is also included.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
*Air pollution *Automobiles *Mathematical models *Advection *Diffusion *Chemical reactions		13B 13F 12A 20M 07D

18. DISTRIBUTION STATEMENT RELEASE TO PUBLIC	19. SECURITY CLASS *(This Report)* UNCLASSIFIED	21. NO. OF PAGES 8
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE A02-A01

EPA Form 2220-1 (9-73)

REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

8

EPA-600/J-77-118
JOURNAL ARTICLE

Reprinted from Preprint Volume: Joint Conference on Applications on Air Pollution Meteorology. Nov. 29-Dec. 2, 1977; Salt Lake City, UT. Published by American Meteorological Society, Boston, ...

A HIGHWAY MODEL FOR THE ADVECTION, DIFFUSION AND CHEMICAL REACTION OF POLLUTANTS RELEASED BY AUTOMOBILES: PART I—Advection And Diffusion Of SF_6 Tracer Gas

Robert E. Eskridge and Kenneth L. Demerjian*

Meteorology and Assessment Division, ESRL
Environmental Protection Agency
Research Triangle Park, North Carolina 27711

1. INTRODUCTION

The problem of automobile pollution has been of interest since the National Environmental Policy Act of 1969, which requires that highways which are partially funded by federal funds have an impact statement before construction begins. The first models developed used steady-state assumptions which yielded Gaussian solutions (see Chen and March, 1970; and Zimmerman and Thompson, 1975): While the Gaussian solution is a reasonable approximation for some situations it encounters difficulties when wind speeds are low and the vertical structure of the atmosphere is important.

The most feasible method of modelling the near highway environment to include chemical kinetics, variable terrain, and vertical variations in the atmosphere is to solve the atmospheric diffusion equation using finite-difference methods. The first attempt to use finite-difference methods is that of Danard(1972). Danard's model suffers from the use of rather large eddy diffusion coefficients and the method of determining K_z is crude. Other models have been developed by Egan et al. (1973), Ragland and Peirce(1973) and Kirsch and Mason(1974). The model of Egan et al. is of interest because it combines the very accurate conservation of moments method for calculating the advection terms with a Gaussian approximation. The model of Ragland and Peirce assumes steady-state conditions and uses a reasonable method of calculating K_z. None of these models includes chemistry, or attempts to parameterize the turbulence of automobiles except in very elementary ways.

A finite-difference model has been developed which overcomes the shortcomings of these models. This model, which is reported here, allows for the inclusion of linear or nonlinear chemical kinetics and uses similarity theory (Flux profile relationships) which have been developed for the surface layer to determine a reference or basic state eddy diffusion coefficient. This first paper is concerned only with the ability of the model to predict the transport and diffusion of SF_6. The chemical aspects of the model will be considered in a later paper.

A review of the GM-sulfate-dispersion experiment and data is presented in section 2. In section 3 the model and boundary conditions are presented, while section 4 addresses the numerical methods and the results are presented in section 5.

2. THE GENERAL MOTORS SULFATE DISPERSION EXPERIMENT

The GM test was held in September and October of 1975 at the GM proving grounds in Milford, Michigan. A fleet of 352 automobiles were driven on a north-south track of 10 km length for seventeen days during the morning hours (see Cadle et al., 1976 for a complete description of the experiments and analysis procedures).

Meteorological instruments and chemical samplers were located on six towers and two stands 2.4 km north of the south end of the test track (see Fig. 1 and 2). Wind speeds from the twenty UVW anemometers were recorded every second. The wind instruments were located on the towers approximately 1.5, 4.4, 10.44 m above the surface and the syringe samplers used to sample SF_6 were located at .5, 3.5, and 9.5 m above the surface. Temperature data were recorded from towers 1 and 6 every five seconds using a Rosemount Model 78-0039-0023 single-element, platinum-resistance thermometer mounted in Model 43404 Gill-aspirated temperature shields. The temperature instruments were located at the same heights as the UVW instruments.

Packs of twenty-two cars were spaced 300 m apart with the lead car traveling 80 km hr^{-1}. Uniformly distributed through the sixteen packs were seven or eight pickup trucks that released SF_6 tracer gas. Sampling began approximately five minutes after the vehicles started around the track. Four sequential samples, each taken over a thirty-minute period, were analyzed for SF_6. Sampling of SF_6 was accomplished using a modified Developmental Science syringe sampler which collected a 30 cm^3 sample in the half hour period. The samplers were analyzed using an automatic dual-column gas chromatograph equipped with electron capture detectors. Analysis accuracy was estimated to be within ± six percent. Problems occurred on two of the days in the release of SF_6, there-

*On assignment to EPA from the National Oceanic and Atmospheric Administration.

fore, the total number of sample periods is 58 instead of 66.

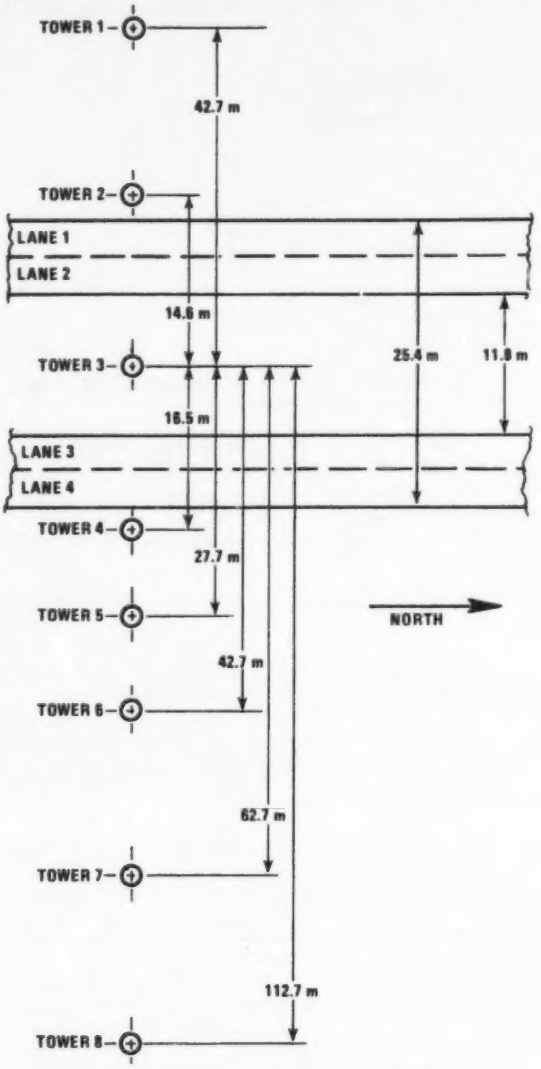

Figure 1. Orientation of test track and perpendicular distances of the meteorological towers from the center of the test track.

3. THE MODEL

Due to the complexity of modelling a roadway with moving vehicles this study will parameterize the effect of the cars as a perturbation eddy diffusion coefficient and add it to a reference eddy diffusion coefficient determined by flux profile relationships for the constant flux layer.

a. The Equation

The general form of a conservation of species equation, neglecting chemical reactions, is

$$\frac{\partial A}{\partial t} = -\nabla_2 \cdot A\vec{V} + \frac{K\partial^2 A}{\partial x^2} + \frac{\partial}{\partial z}\frac{K\partial A}{\partial z} + E(\vec{x},t), \qquad (1)$$

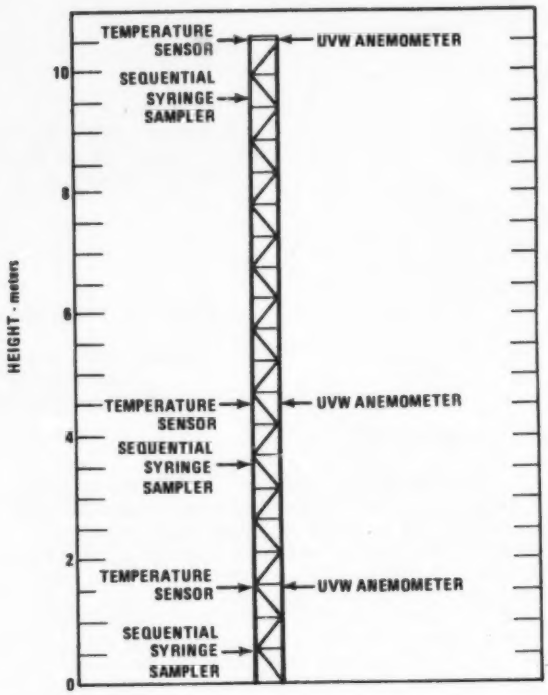

Figure 2. Nominal height of instruments above the ground for the six towers.

where ∇_2 is the divergence operator in the x and z coordinates, E(x,t) is an emission source term, K is the eddy diffusion coefficient determined by flux profile relationships, and A is some chemical species.

A primary assumption in this model is that a basic or undisturbed atmosphere exists on which the effects of the roadway are imposed as an additive effect. In the GM experiment, vertical wind shear and temperature gradients are available and therefore, eddy diffusion coefficients can be calculated in the vertical using flux profile relationships. The Richardson number is calculated by

$$R_i = \frac{\frac{g}{T}\left(\frac{\partial T}{\partial z} + \frac{g}{c_p}\right)}{\left(\frac{\partial u}{\partial z}\right)^2} \qquad (2)$$

The vertical eddy diffusion coefficients are then calculated using the following equations which are taken from Dyer(1974):

$$\zeta = R_i/(1-5R_i) \quad R_i \geq 0, \quad \zeta = R_i \quad R_i < 0 \qquad (3)$$

$$R_i < 0 \quad \chi = (1-16\zeta)^{1/4}, \quad \psi = \ln(1+\chi)^2 (1+\chi^2)/8 - 2\tan^{-1}(\chi) + \pi/4 \qquad (4)$$

$$R_i \geq 0 \quad \chi = -5\zeta$$

$$u_* = k\, u(z)/\ln(z/z_0) - \psi \qquad (5)$$

$$\phi_m(\zeta) = (1-16\zeta)^{-1/4} \quad R_i < 0$$

$$\phi_m(\zeta) = 1 + 5\zeta \qquad R_i \geq 0 \qquad (6)$$

$$K_m(z) = \frac{kzu_*}{\phi_m(\zeta)} \qquad (7)$$

The procedure for determining $K_m(z)$ is to first calculate R_i using (2), then ζ (i.e. z/L) can be estimated using (3) which is different depending on whether the atmosphere is stable or unstable. The friction velocity u_* can then be calculated using (4) and z_0, which was determined to be 1.35 cm. At this point $K_m(z)$ can be calculated by (7) using (6) and the value of u_* from (5).

It has been assumed that pollutants diffuse in the same manner as momentum. While the diffusion of water vapor might likely be a more reasonable analogue, the functions describing the diffusion of water vapor are not well known.

There has been some analysis work of the wakes of single vehicles (Fay,1973), but very little is known of the effect of multiple wakes. Therefore a wake eddy diffusion coefficient profile was determined using one thirty minute period of data from the GM test. A period of perpendicular and very stable flow ($R_i > .25$) was chosen to calculate the wake eddy diffusion profile. This profile (Fig. 3) is a maximum near the surface and decreases rapidly as a function of height and is zero at 13.5m above the roadway. It is also assumed that K', the wake eddy diffusion coefficient, decreases linearly with vehicle speed and, is zero when the vehicle speed is zero.

The conservation of species equation becomes

$$\frac{\partial A}{\partial t} = -\nabla_2 \cdot A\vec{V} + K_x \frac{\partial^2 A}{\partial x^2} + \frac{\partial}{\partial z} K^* \frac{\partial A}{\partial z} + E(\vec{x},t) \qquad (8)$$

where $K^* = K_m + K'$, and $K_x = 5\,K^*$.

b. The Boundary Conditions

The problem of imposing boundary conditions is always difficult in the atmosphere especially when the scale of the problem is small.

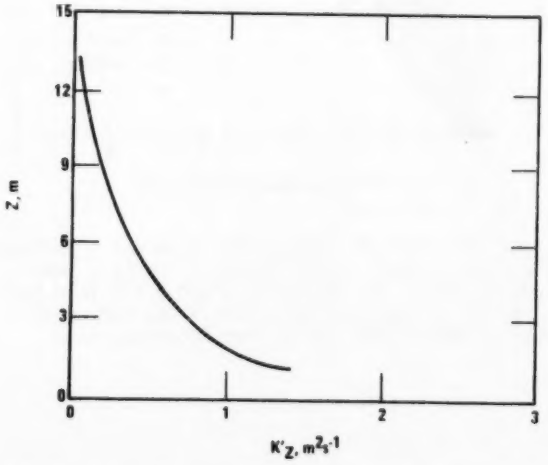

Figure 3. The vertical variation of the wake eddy diffusion coefficient for vehicle speed of 80 km hr^{-1}.

In this model it is assumed that the gradient at the surface is zero, which represents

$$\frac{\partial A}{\partial z} = 0 \quad \text{at } z = 0, \qquad (9)$$

no loses at that boundary. At the side boundaries the zero gradient condition

$$\frac{\partial A}{\partial x} = 0 \quad \text{at } x = 0 \text{ and } x = x_{max}, \qquad (10)$$

is also imposed. At the top it is assumed that the concentration is zero

$$A = 0 \text{ at } z = z_{max}. \qquad (11)$$

These boundary conditions are not without problems as they are imposed only for mathematical reasons. It has been found in experimentation that the model results were more sensitive to the height of the modelling region than to any of the boundary conditions. Therefore, when the winds are light or parallel to the roadway the height of the integration region is raised to 90 meters.

4. THE NUMERICAL PROCEDURE

a. The Grid

The numerical solution of equation (1) requires that it be expressed in finite differences on some grid. For this problem all of the variables are defined at each grid point. The grid lengths were chosen so that in the x direction Δx is equal to the width of one traffic lane and $\Delta z/2$ is approximately the height of an automobile.

b. The Numerical Scheme

Equation (1) can be written in operator form as

$$\frac{\partial A}{\partial t} + B_1 A + B_2 A = B_3 A + B_4 A + E, \qquad (12)$$

where B_1, B_2, B_3, and B_4 are linear operators. Equation (12) can be approximated by

$$\frac{A^{n+1} - A^n}{\Delta t} + \Lambda_1 A_{ik} + \Lambda_2 A_{ik} = \Lambda_3 A_{ik} + \Lambda_4 A_{ik} + E_{ik}, \qquad (13)$$

where Λ_i, $i = 1,\cdots,4$ are approximations of B_i. Equation (13) will be solved by a type of fractional step method (see Marchuk, 1975 for a complete descriptions of the method of fractional steps). The procedure is as follows:

$$A^1 = A^n + \Delta t\, \Lambda_1 A^n, \qquad (14)$$

$$A^2 = A^1 + \Delta t\, \Lambda_2 A^1, \qquad (15)$$

$$A^3 = A^2 + \Delta t\, \Lambda_3 A^2, \qquad (16)$$

$$A^4 = A^3 + \Delta t\, \Lambda_4 A^3, \qquad (17)$$

$$A^{n+1} = A^4 + \Delta t\, E_{ik}. \qquad (18)$$

If one eliminates $A^1,\cdots,A^4$ the system reduces to an equation of the form

$$A^{n+1} = A^n + \Delta t(\Sigma\Lambda_i)\, A^n + \Delta t\, E_{ik} + (\Delta t)^2(\cdots\cdot)$$

$$+ (\Delta t)^3 + \text{higher order terms.} \qquad (19)$$

The operators Λ_3, Λ_4 are simply centered in space approximations, while the operators Λ_1, Λ_2 which solve the flux terms are based on a flux-corrected algorithm of Zalesak (1976). This algorithm is an upstream scheme which insures positive

values for the concentration at every grid point. This is important, since Eskridge and Demerjian (1977) have shown that negative concentrations combined with nonlinear chemistry can result in unstable numerical schemes. The algorithm also reduces numerical diffusion and is stable for

$$\Delta t \leq 1/2 \frac{\Delta x}{u_{max}} .$$

Because of the complexity of this algorithm we have been unable to show that the fractional step procedure is compatible with the original differential equation. However, if just an upstream approximation is used to calculate the flux terms it can be shown that the truncation error (the difference between the partial differential equation and the approximation) is

$$O(\Delta t) + O(\Delta x) + O(\Delta t/\Delta x). \qquad (20)$$

The complexity of the flux algorithm also prevents us from establishing that the procedure is stable. Experience has shown that if every separate step is stable, the calculation is stable.

The upstream algorithm, while not as accurate as a centered scheme, such as SHASTA (Boris and Book,1973), has the advantage of requiring only one point outside the integration region for boundary conditions.

5. THE RESULTS

The model was run to simulate highway emissions for fifty one-half hour periods and the results are shown in figures 4 through 8. Figures 4 and 5 are scatter diagrams of the observations vs. prediction of the finite-difference model and the EPA highway model(Petersen,1976), respectively. Comparison of these two figures shows that the finite-difference model does a better job of predicting the maximum values observed in the GM experiment. One also notices that the slope of the linear least squares fit line is much closer to one and the correlation is higher for the finite-difference model than the EPA Gaussian model.

In figure 6 the correlation between observation and prediction for each station is shown for all time. The station numbers indicated the tower (see figure 1) and level above the surface. Station 1 is located on tower 1 at 10.5m, station 2 is located on tower 1 at 4.5m and station 3 is located on tower 1 at 1.5m and so on. This figure shows the correlation to be highest near the roadway and to decrease with increase of distance away from the roadway.

Figure 7 is a plot of the correlation between observations and predictions for the network for each half hour period. The correlation is generally very high and decreases in the last 12 periods. Periods 38 through 50 represent the periods of light winds, and stable conditions.

Figure 8 is a frequency distribution plot of (O-P)/O, where O represents observation and P represents prediction. Ideally this figure would be Gaussian indicating that the errors are random. This plot is not Gaussian, but does indicate that there is no particular bias in the predictions.

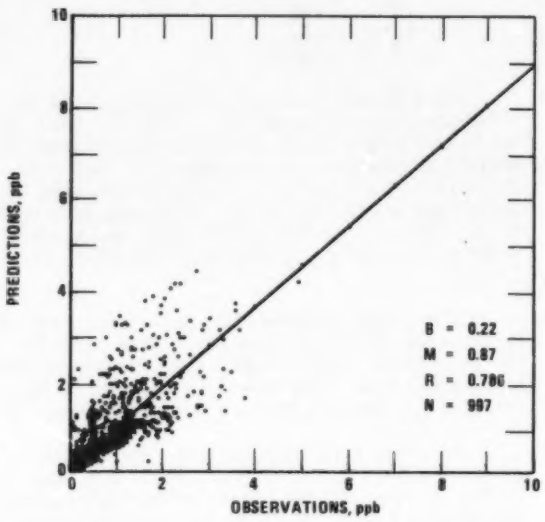

Figure 4. Plot of computed vs. observed SF_6 using finite difference model. The straight line is a least square linear fit with slope M and intercept B; R is the correlation and N the number of data points.

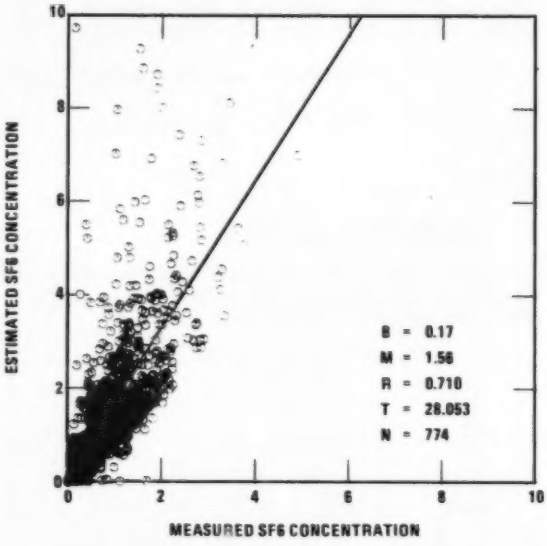

Figure 5. Plot of computed vs. observed SF_6 using EPA highway model. The straight line is a least squares fit to the data with slope M and intercept of B. R is the correlation and N the number of data points. This figure from Petersen, 1976.

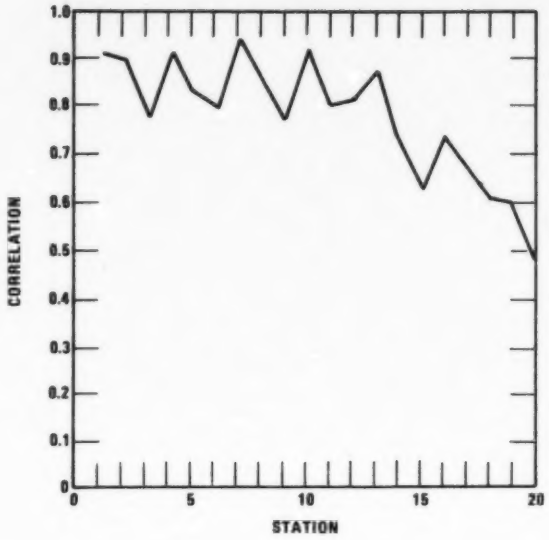

Figure 6. Plot of the correlation at each station for all experiments.

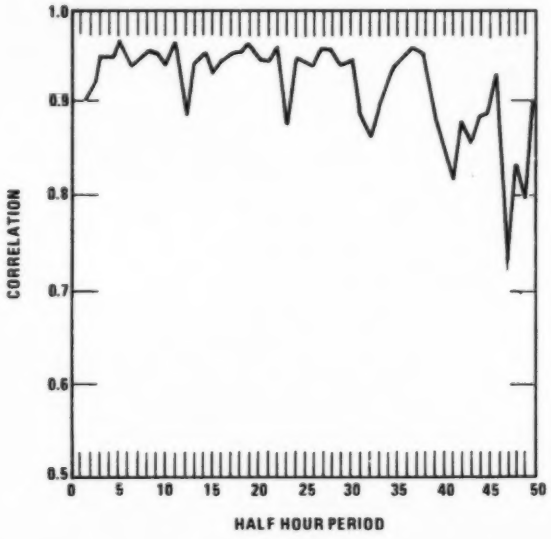

Figure 7. Plot of the correlation between observation and prediction at the twenty stations for each half hour period.

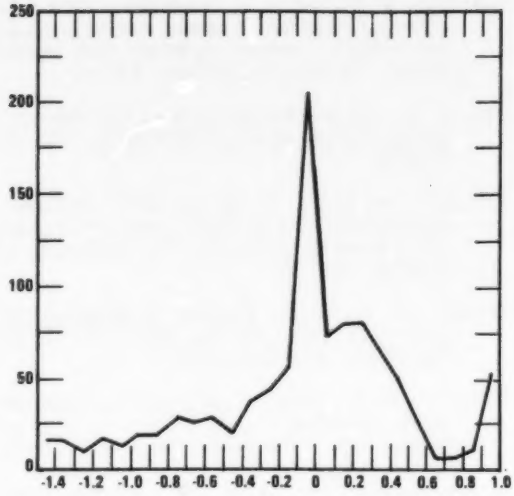

Figure 8. Plot of frequency distribution of O-P/O for intervals of .1.

6. CONCLUSION

This paper presented a finite-difference model of a highway which includes surface layer physics and a parameterization of the wake effect of automobiles. This model was shown to produce better results than the EPA highway model. Analysis of the model shows that the accuracy decreases with increase of distance from the highway, that it does not predict as well when the winds are light, and that the errors are evenly distributed.

7. REFERENCES

Boris, J. P. and D. L. Book, 1973: Flux-corrected transport. I. SHASTA, A fluid transport algorithm that works. J. Comp. Physics., 11, 38-69.

Cadle, S. H., D. P. Chock, J. M. Heuss, and P. R. Monson, 1976: Results of the General Motors sulfate dispersion experiments. General Motors Research Publication GMR-2107, Warren, Michigan. 140 pp.

Chen, T. C. and F. March, 1970: Effect of highway configurations on environmental problems-dynamics of highway associated air pollution. Second International Clean Air Congress, 35-40.

Danard, M. B., 1972: Numerical Modelling of carbon monoxide concentrations near highways. J. Appl. Meteor., 11, 947-957.

Dyer, A. J., 1974: A review of flux-profile relationships. Boundary Layer Meteor., 7, 363-372.

Egan, B. A., A. Epstein and M. Keefe, 1973: Development of procedures to simulate motor vehicle pollution levels. Final Report, D. C. Department of Highways and Traffic. NTIS PB-233-938.

Eskridge, R. E. and K. L. Demerjian, 1977: Evaluation of numerical schemes for solving a conservation of species equation with chemical terms. To appear in Atmos. Envir.

Fay, J. A., 1973: Buoyant plumes and wakes. Annual Review of Fluid Mechanics, VOL. 5, 151-160.

Kirsch, J. W. and B. F. Mason, 1974: EXPLOR-examination of pollution levels of roadways. Final Report, California Air Resources Board. NTIS PB-236-713.

Marchuk, G. I., 1975: Methods of Numerical Mathematics Springer Verlag, New York, 316 pp. Translated by Jiri Ruzicka.

Petersen, W. B., 1976: Comparison of dispersion model estimates with measured sulfate concentrations. The General Motors/Environmental Protection Agency sulfate dispersion experiment - selected EPA research papers. Report EPA 600/3-76-035, Research Triangle Park, N. C., 149 pp.

Ragland, K. W. and J. J. Peirce, 1973: Air pollution due to highway traffic. Working paper 13, University of Wisconsin. NTIS PB-228-691.

Zalesak, S. Personnal communication.

Zimmerman, J. R. and R. S. Thompson, 1975: User's guide for Hiway, a highway air pollution model. EPA report EPA-650/4-74-008.